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Abstract. Standardized formats for atomic data used in calculating emission from a collisionally-ionized plasma are described. The formats use the astronomical-standard FITS format, and are extendible to other purposes, such as photoionization data. The formats emphasize storing references to the original data source and keeping the data in as-received form, to aid in checking against the original literature.

1. Introduction

Calculating the spectrum of a thermal plasma remains an ongoing challenge involving both atomic and plasma physics, as well as numerical computational issues. We have been working on a new code called the Astrophysical Plasma Emission Code (*APEC*), which separates these issues so they can be attacked individually. *APEC* contains no atomic data, but calculates the emission from a hot plasma using atomic data stored in the Astrophysical Plasma Emission Database (*APED*). Many atomic processes, including radiative recombination, dielectronic recombination and satellite lines, and collisional de-excitation, are included in a self-consistent fashion. This approach has the advantage, for example, of including the density dependence of each transition.

Although the majority of our time was spent developing the *APEC* code, the longer-term aspect of this project is the continuing development of the atomic database *APED*. *APED* files are stored as binary tables using the FITS (Flexible Image Transport System) format, which has been used for astronomical data storage and transfer since 1979. FITS files are formatted into blocks of

data called Header Data Units (HDUs). Each HDU contains an ASCII header which describes the data to follow, and some data (either an image or a table). The FITS format is an International Astronomical Union standard, and is described in detail at `http://fits.gsfc.nasa.gov/`. We chose to use the FITS format because it is compact, familiar to astronomers, and portable across many different software packages.

The latest version of the *APED*, along with the most recent collisional ionization calculation from *APEC*, can be found at `http://hea-www.harvard.edu/APEC/ATOMDB/`.

2. APED Formats

The data in the APED are organized in one of four different table types, depending on the physical process involved. In general, each process and ion is stored in a separate file, although this is not required–each HDU is independent, so it would be possible to bundle data together into a single file if desired.

The type of an HDU block in a FITS file is set in the header keyword HDUCLASS, and any subcategory is set in HDUCLASn keywords. All the HDUs in the *APED* have HDUCLASS set to ATOMIC. In addition, we use the NASA Goddard checksum convention[1] to uniquely mark each HDU. The values of each checksum used in a given *APEC* run are carried into the *APEC* output so that the exact atomic data used for any aspect of the calculation can be identified.

2.1. Energy Levels

An energy level HDU has HDUCLAS1 set equal to E_LEVEL. Each row of the table contains data for a single energy level, as described in Table 1. The row order is normally ground state first, and then in increasing energy. However, neither the row nor column order is significant. If data is not available–for example, the spin quantum number–an explicit NULL value is used. The photoionization data is stored for the purposes of calculating the radiative recombination continuum; we need to extend the format to include innershell ionization for use with photoionization codes. The current parameterizations (for PHOT_TYPE) are -1 for no photoionization, 0 for hydrogenic, 1 for data from Clark, Cowan, & Bobrowicz (1986), and 2 for data from Verner & Yakovlev (1995). All references are stored as bibcodes, a short human- and machine-readable format (Schmitz, 1995).

2.2. Radiative Transitions

The radiative transition file has HDUCLAS1 set to EM_LINES. Each row of the file (see Table 2) gives the transition rate for a particular transition from one level to another. The level indices begin at 1, and use the same row order as is used in the energy level table for the ion. Two levels $j \rightarrow i$ may have more than one listing, for example if both the electric dipole and magnetic quadrupole were calculated separately. *APEC* will simply sum the rates together. The rationale for keeping identical transitions separate is to aid in checking against the original

[1] http://heasarc.gsfc.nasa.gov/docs/heasarc/ofwg/docs/general/checksum/checksum.html

Table 1. Energy Level Table Format

Column	Units	Data Type	Description
ELEC_CONFIG		String[40]	Electonic configuration, preferably in TeX format
ENERGY	eV	Real4	Energy of level (ground state = 0 eV)
E_ERROR	eV	Real4	Error in level energy, if available
N_QUAN		Int4	Principal quantum number of outermost electron
L_QUAN		Int4	Angular momentum of level
S_QUAN		Real4	Spin quantum number of level
LEV_DEG		Int4	Statistical weight of level
PHOT_TYPE		Int4	Type of photoionization data
PHOT_PAR[20]		Real4(20)	Photoionization cross section of the outermost electron
ENERGY_REF		String[20]	Reference for energy of level
PHOT_REF		String[20]	Reference for photoionization data

data source. We also keep up to two wavelengths for each transition; for the majority of our transitions we have only a theoretical wavelength, but when available the observed wavelength is preferred. In the final output file, however, *APEC* gives only one wavelength.

Table 2. Radiative Transition Format

Column	Units	Data Type	Description
UPPER_LEV		Int4	Transition's upper level, from energy level file
LOWER_LEV		Int4	Transition's lower level, from energy level file
WAVELEN	Angstrom	Real4	Theoretical wavelength
WAVE_OBS	Angstrom	Real4	Observed wavelength (preferred)
WAVE_ERR	Angstrom	Real4	Error on observed wavelength
EINSTEIN_A	s**-1	Real4	Transition rate
EIN_A_ERR	s**-1	Real4	Error on transition rate
WAVE_REF		String[20]	Reference for th. wavelength
WV_OBS_REF		String[20]	Reference for observed wavelength
EIN_A_REF		String[20]	Reference for transition rate

2.3. Collisional Excitation

The collisional excitation file format (see Table 3) covers both electron and proton excitation; in both cases, HDUCLAS1 is set to COLL_STR. The trickiest aspect is the parameterization of the collision strength data. A number of different approaches are used in the literature, and since one of *APED*'s goals is to use the data as published (or received), we have to implement many methods. Table 4 lists the possible values for the COEFF_TYPE parameter; both effective collision strengths (Υ) and rate coefficients (q) are stored in this format. Types which use interpolation store the temperatures in the TEMPERATURE column; otherwise, this column is ignored. For interpolated data with N data points, the coefficient type used is the base value plus N. Thus, interpolated electron effective collision strength data with 16 points over a closed interval should have COEFF_TYPE=116; 13 points of proton excitation rates over an open inter-

val would have COEFF_TYPE=463. The maximum number of parameters (or interpolation points) is set to 20 by definition. Just as in the radiative transition file, multiple rows with identical upper and lower levels are allowed. So, if more data need to be stored, multiple rows can be used with the appropriate MIN_TEMP, MAX_TEMP range.

Table 3. Collisional Excitation Format

Column	Units	Data Type	Description
LOWER_LEV		Int4	Transition's upper level, from energy level file
UPPER_LEV		Int4	Transition's lower level, from energy level file
COEFF_TYPE		Int4	The type of parameterization; see Table 4
MIN_TEMP	K	Real4	Minimum temperature of applicability
MAX_TEMP	K	Real4	Maximum temperature of applicability
TEMPERATURE[20]	K	Real4(20)	Temperature array
EFFCOLLSTRPAR[20]		Real4(20)	Effective collision strength parameters
REFERENCE		String[20]	Reference for effective collision strength

2.4. Dielectronic Recombination

For dielectronic recombination (see Table 5), we use the DR_LINES for the HDUCLAS1 keyword. We also use the isolated resonance approximation (ISA), which has DR_TYPE=1, as this is how most of the data are available. However, we are open to defining new types as more data become available. The only other issue is that since dielectronic recombination links two ion states, there is always a certain amount of confusion. In *APED*, the dielectronic recombination data linking parent ion to daughter ion is lists the parent state in the header, but the upper and lower levels refer to the daughter ion's levels. Thus, the data for satellites to O VIII is stored in the O VIII directory, but refers to O VII levels. In addition, only the LOWER_LEV is required to exist as an actual level in the daughter energy level file; the doubly-excited upper state may not explicitly exist, as it is only populated by dielectronic recombination. Non-existent upper levels are given values above 10,000 to distinguish them from real levels.

3. Conclusions

These atomic data formats allow astronomers easy access to the data and its references. Standard X-ray astrophysics packages such as Sherpa, XSPEC, and ISIS already use the *APED*, and as astronomers become more used to high-resolution X-ray spectroscopy, we expect *APED* use to grow dramatically. More information about *APEC*, *APED*, and projects using them is avaiable at `http://hea-www.harvard.edu/APEC/`.

References

Clark, R. E. H., Cowan, R. D. & Bobrowicz, F. W. 1986, ADNDT, 34, 415

Dere, K. P., Landi, E., Mason, H. E., Monsignori Fossi, B. C., & Young, P. R. 1997, A&AS, 125, 149

Table 4. Collision Strength Parameterizations

Value	Type	Description
11	e, Υ	Chianti type 1 (see Dere *et al.*1997)
12	e, Υ	Chianti type 2 (see Dere *et al.*1997)
13	e, Υ	Chianti type 3 (see Dere *et al.*1997)
14	e, Υ	Chianti type 4 (see Dere *et al.*1997)
31	e, Υ	Sampson, Goett & Clark (1983) fit type 1
32	e, Υ	Sampson, Goett & Clark (1983) fit type 2
33	e, Υ	Sampson, Goett & Clark (1983) fit type 3
41	e, Υ	Kato & Nakazaki (1989) fit type 1
42	e, Υ	Kato & Nakazaki (1989) fit type 2
100+N	e, Υ	Interpolation; max/min values are both usable
150+N	e, Υ	Interpolation; max/min values are not used
200+N	p, Υ	Interpolation; max/min values are both usable
250+N	p, Υ	Interpolation; max/min values are not used
300+N	e, q	Interpolation; max/min values are both usable
350+N	e, q	Interpolation; max/min values are not used
400+N	p, q	Interpolation; max/min values are both usable
450+N	p, q	Interpolation; max/min values are not used
500+N	e, Υ	Interpolation; use min, not max
550+N	e, Υ	Interpolation; use max, not min
600+N	p, Υ	Interpolation; use min, not max
650+N	p, Υ	Interpolation; use max, not min
700+N	e, q	Interpolation; use min, not max
750+N	e, q	Interpolation; use max, not min
800+N	p, q	Interpolation; use min, not max
850+N	p, q	Interpolation; use max, not min

Table 5. Dielectronic Recombination Format

Column	Units	Data Type	Description
UPPER_LEV		Int4	Transition's upper level, from daughter ion's energy level
LOWER_LEV		Int4	Transition's lower level, from daughter ion's energy levels
WAVELEN	Angstrom	Real4	Theoretical wavelength
WAVE_OBS	Angstrom	Real4	Observed wavelength
WAVE_ERR	Angstrom	Real4	Error on observed wavelength
DR_TYPE		Int4	Type of DR data; = 1 for IRA
E_EXCITE	keV	Real4	Excitation energy for DR satellite
EEXC_ERR	keV	Real4	Error on excitation energy
SATELINT	s**-1	Real4	Satellite rate
SATINTERR	s**-1	Real4	Error on satellite rate
PARAMS[10]		Real4(10)	To be used by non-ISA data
DRRATE_REF		String[20]	Reference for satellite rate
WAVE_REF		String[20]	Reference for theoretical wavelength
WV_OBS_REF		String[20]	Reference for observed wavelength

Kato, T. & Nakazaki, S. 1989, ADNDT, 42, 313

Sampson, D. H., Goett, S. J. & Clark, R. E. H. 1983, ADNDT, 29, 467

Smith, R. K., Brickhouse, N. S., Liedahl, D. A. & Raymond, J. C. ApJL, submitted.

Schmitz, M., Helou, G., Dubois P., LaGue C., Madore B., Corwin Jr, H. G. & Lesteven, S., 1995, in "Information & On-line Data in Astronomy", eds. D. Egret & M.A. Albrecht, (Kluwer Acad. Publ.), p. 259.

Verner, D. A. & Yakovlev, D. G. 1995, A&AS, 109, 125

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